Design of Phosphorus-Containing MWIR Type-II Superlattices for Infrared Photon Detectors

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***Abstract*—Type-II strained layer superlattices (SLSs) offer a broad range of design degrees of freedom to help optimize their properties as absorber layers of infrared photon detectors. We theoretically examine a new class of mid-wavelength infrared (2–5 μm bandpass) Type-II structures with two-layer InGaSb/InPSb and four-layer InAs/GaSb/InAs/InPSb SLS periods. Phosphorous-containing SLSs are a promising approach to improving infrared photon detector performance due to providing a new set of material properties, including favorable valence band offsets. P-based SLSs of four-layer type InAs/GaSb/InAs/InPSb were found to be among the best 5-μm gap SLSs that we have modeled. Among the studied designs, the lowest dark current in an ideal structure is predicted for a four-layer 23.6 Å InAs/20 Å GaSb/23.6 Å InAs/60 Å $InP_{0.62}Sb_{0.38}$ SLS. Its predicted ideal dark current is about 35 times lower than an n-type HgCdTe-based photodiode absorber and six times lower than a p-type HgCdTe one for the same bandgap, temperature, and dopant concentration. We also discuss a defect mitigation strategy that involves positioning the SLS gap in an energy range that avoids defect levels and show how this applies to the aforementioned P-containing SLS.**

***Index Terms*—Auger recombination, detector, infrared, Type-II superlattice.**

I. Introduction

HIGH-quality, high-operating temperature infrared photodiodes based on HgCdTe are typically limited in sensitivity by Auger recombination in their absorber layers [1].

Type-II strained layer superlattices (SLSs) based on InAs/GaInSb are of interest in part because they offer the possibility to design features into their electronic band structures that reduce the rate of Auger recombination, for example, by reducing the density of available final states. The ability of the InAs/GaSb material system to achieve small infrared energy gaps was first predicted in 1977 [2]. Its theoretical proposal as a high performing material system for infrared detection was made in 1987 [3], suggesting optical absorption similar to that of HgCdTe alloys and effective masses that lead to favorable electrical properties, such as low photovoltaic device tunneling currents and good carrier mobility. The experimental realization of infrared energy gaps and optical absorption comparable to HgCdTe took place in 1990 [4]. Theoretical predictions of Auger lifetimes orders of magnitude longer in InAs/GaInSb SLS than in HgCdTe alloys were made in 1992 [5] and confirmed experimentally with photoconductive response measurements in 1994 [6].

Designing an SLS to exhibit Auger suppression via final state optimization becomes more challenging as the SLS bandgap increases due to the increasing number of SLS subbands that exist in critical final state regions of the electronic band structure [7]. Mid-wavelength infrared (MWIR) SLSs are therefore particularly challenging to optimize. To our knowledge, this is the first quantitative consideration of P-containing Type-II SLS for infrared detector applications. We initially examined SLS absorber layers of the form GaSb/InPSb (containing two-layer per SLS period), where the InPSb layer was lattice-matched to GaSb, but were unable to reach a 5-μm bandgap at 200 K. Turning to InGaSb/InPSb, with strained InPSb and a strain-balanced unit cell, gave the freedom to reach the desired bandgap. We then examined P-containing SLS designs with four layers per period, which are predicted to exhibit substantially better device performance. The latter two classes are discussed in the following. In addition, we suggest a strategy to mitigate the deleterious effects of defects in mediating recombination that is currently limiting the performance of Type-II SLS-based photodetectors.

II. Electronic Structure

The SLSs were designed to possess a 5-μm bandgap wavelength at 200 K. The calculations of the electronic band structure are based on a 14-band bulk basis for the III–V constituents of the SLS, and an envelope-function-based SLS **K•p** formalism [8]. The SLS is considered to be a highly anisotropic periodic structure. The zone-center states are calculated in Fourier space using a 14-band basis for the envelope functions. The need to rely on a 14-band basis rather than the more common eight-band basis arises because of the sensitivity of the optical and electronic properties to the electronic structure in the secondary regions of the band structure. Errors inherent

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14. ABSTRACT

Type-II strained layer superlattices (SLSs) offer a broad range of design degrees of freedom to help optimize their properties as absorber layers of infrared photon detectors.We theoretically examine a new class of mid-wavelength infrared (2?5 μm bandpass) Type-II structures with two-layer InGaSb/InPSb and four-layer InAs/GaSb/InAs/InPSb SLS periods. Phosphorouscontaining SLSs are a promising approach to improving infrared photon detector performance due to providing a new set of material properties, including favorable valence band offsets. P-based SLSs of four-layer type InAs/GaSb/InAs/InPSb were found to be among the best 5-μm gap SLSs that we have modeled. Among the studied designs, the lowest dark current in an ideal structure is predicted for a four-layer 23.6 ? A InAs/20 ?A GaSb/23.6 ?A InAs/60 A? InP0.62Sb0.38 SLS. Its predicted ideal dark current is about 35 times lower than an n-type HgCdTe-based photodiode absorber and six times lower than a p-type HgCdTe one for the same bandgap, temperature, and dopant concentration. We also discuss a defect mitigation strategy that involves positioning the SLS gap in an energy range that avoids defect levels and show how this applies to the aforementioned P-containing SLS.

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in the eight-band model become significantly more pronounced as the states one is interested in become farther from the band edge. This is particularly relevant in MWIR structures relative to longer wavelength ones.

The use of Fourier space to solve the envelope function equations at the zone center avoids the issues associated with matching conditions at sharp interfaces and also provides a sensible way to choose a balanced basis set for the SLS **K•p** calculations. Momentum matrix elements are then evaluated among these SLS states, and a **K•p** calculation using the SLS states is performed. We have checked the convergence of the **K•p** calculations by increasing the number of Fourier terms up to the point where the highest order term has a wavelength of order the atomic spacing, and confirmed that the results do not change.

III. Computation of Optical Absorption and Recombination Rates

SLS optical absorption coefficients were computed directly from the SLS **K•p** energy bands and matrix elements. The absorption spectrum of HgCdTe was obtained from semiempirical equation (7) in [9] and will be employed later in the computation of dark currents for comparison with the SLS.

Auger recombination rate calculations, which are computationally more intensive, require additional approximations and are thus characteristically less accurate than optical properties. The highly nonparabolic band structures and momentum matrix elements are used directly as input for the computation of SLS Auger lifetimes. They are input into the Auger rate computations in the form of lookup tables with a mesh spacing of 0.002 Å^{-1}. The principal methods employed are discussed in [7], and have been extended to include the effects of SLS Umklapp processes [10], which have shown to contribute approximately half of the total rate of Auger recombination in SLS. The transition matrix elements are evaluated using a statically screened Coulomb interaction and first-order **K•p** for the wave function overlaps. The multidimensional K-space integrals are evaluated employing an adaptive mesh Monte Carlo algorithm. For HgCdTe, the Auger lifetimes were computed from the Blakemore expression [11] with $|F_1 F_2| = 0.2$ and $\gamma = 6$. Both Auger-7 and Auger-1 recombination mechanisms were included in all cases.

Radiative recombination is not included in the calculations due to Humphrey's [12] suggestion that standard radiative lifetime estimates, such as those obtained by the van Roosbroeck–Shockley expression [13], are significantly underestimated. Defect-mediated recombination is not included in the calculations. Actual lifetimes are expected to be shorter than those predicted here due to the presence of recombination-mediating defects (see Section VI).

IV. Computation of Ideal Photodiode Dark Currents

A valuable means of comparing the potential performance of various infrared photon detectors is by estimating their dark currents. We computed the diffusion-limited dark currents of the examined Type-II SLS- and, for reference, HgCdTe-based absorber layer photodiodes using the expression:

$$eG_{\text{th}} = e\frac{n_{\min} d}{\tau_A} \tag{1}$$

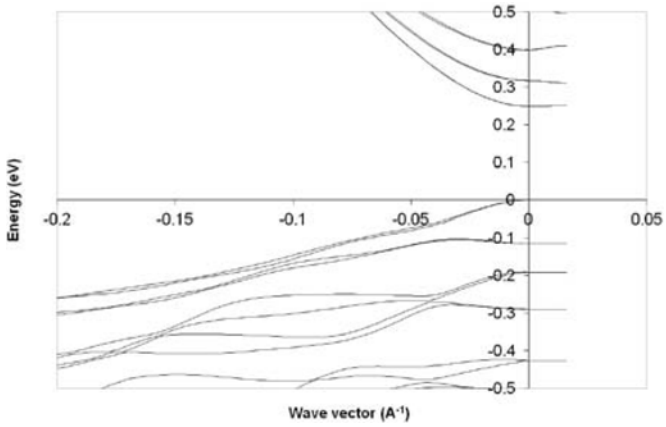

Fig. 1. Computed 200 K electronic band structure of a two-layer 56 Å $In_{0.22}Ga_{0.78}Sb$/160 Å $InP_{0.68}Sb_{0.32}$ SLS at 200 K. Negative wave vectors correspond to the in-plane direction and positive ones to the growth-axis direction.

where e is the electron charge, G_{th} is the thermal generation rate, $n_{\min}$ is the minority carrier concentration, d is the absorber layer physical thickness (assumed to be less than the minority carrier diffusion length), and τ_A is the minority carrier Auger lifetime. This expression considers only the diffusion current coming from absorber region, and as such represents the lowest possible dark current from a classical p-n photodiode (and indeed also an nBn-based device [14]).

To facilitate comparisons between the SLS and HgCdTe, we consider for each material system a 5-μm bandgap and a 200 K operating temperature. The parameters in (1) were obtained as follows. The minority carrier concentrations $n_{\min}$ of the SLS were computed directly from the electronic band structure as obtained using the SLS **K•p** method using Fermi statistics at the temperature under consideration. This method is described in Grein *et al*. [7], with the specific material parameters and calculations described in [8]. P-type dopant concentrations of 1×10^{15}, 1×10^{16}, and 1×10^{17} cm^{-3} with all acceptors singly ionized were considered. The minority carrier concentrations of the HgCdTe alloys were computed employing the Hansen and Schmit expression [15]. For HgCdTe, we considered separately p-type dopant concentrations of 1×10^{15}, 1×10^{16}, and 1×10^{17} cm^{-3}, and n-type dopant concentrations of 1×10^{15}, 1×10^{16}, and 1×10^{17} cm^{-3}. d was chosen to be 5 μm for the HgCdTe absorber (corresponding to a 10 μm optical thickness for a perfectly reflecting contact giving a double pass of the infrared radiation). The absorption coefficient α of all considered SLS and HgCdTe cases was taken to be the absorption coefficient at 9/10 of the gap wavelength λ_g. d for the SLS was computed to give the same αd product as HgCdTe.

V. Results for Ideal Superlattices

A. 56 Å $In_{0.22}Ga_{0.78}Sb$/160 Å $InP_{0.68}Sb_{0.32}$ Two-Layer SLS

The computed 200 K electronic band structure of 56 Å $In_{0.22}Ga_{0.78}Sb$/160 Å $InP_{0.68}Sb_{0.32}$ SLS, which is strain balanced to a GaSb substrate, is shown in Fig. 1. It is predicted to have a 249.3-meV (4.97 μm) bandgap. Its long period is due to the need to minimize quantum confinement energies to realize

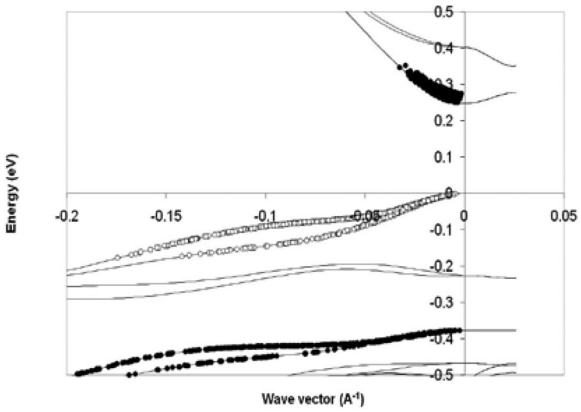

Fig. 2. Computed electronic band structure of a four-layer 23.6 Å InAs/20 Å GaSb/23.6 Å InAs/60 Å $InP_{0.62}Sb_{0.38}$ SLS at 200 K. The electrons (solid circles) and holes (hollow circles) involved in the (roughly) 400 most probable hole–hole Auger transitions at 200 K and p = 1×10^{15} cm^{-3} are also shown. Negative wave vectors correspond to the in-plane direction and positive ones to the growth-axis direction.

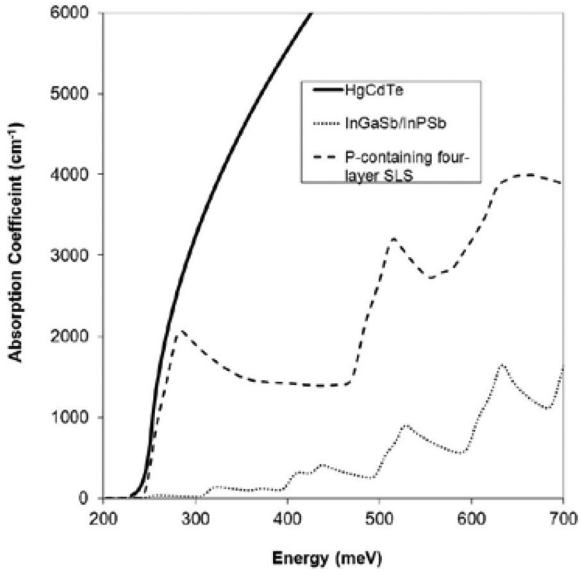

Fig. 3. Computed 200 K optical absorption coefficient of the two-layer 56 Å $In_{0.22}Ga_{0.78}Sb$/160 Å $InP_{0.68}Sb_{0.32}$ ("InGaSb/InPSb") compared with bulk $Hg_{0.715}Cd_{0.285}Te$[9] and four-layer 23.6 Å InAs/20 Å GaSb/23.6 Å InAs/60 Å $InP_{0.62}Sb_{0.38}$ ("P-containing four-layer SLS").

an MWIR gap, which is associated with the fact that the band alignment is staggered Type II and not broken gap Type II like it is for InAs/GaSb-based SLS [16]. Not surprisingly, the long period for this Type-II SLS with only two layers in a period results in weak electron–hole overlaps and hence weak optical absorption. For a p-type dopant concentration of 1×10^{15} cm^{-3} and a temperature of 200 K, we compute a hole–hole Auger (Auger-7) lifetime of 9.8×10^{-3}s (Auger coefficient $\gamma_{3\mathrm{hh}} = 1.0 \times 10^{-28}$ cm^6/s). This low Auger coefficient results from the weak overlap matrix elements, which are similar to those that enter into the optical absorption. As such, while this structure is expected to exhibit weak Auger recombination, it is not of practical value as an infrared photodiode absorber layer due to its weak absorption requiring very thick absorber layers (and very long diffusion lengths) to achieve significant quantum efficiency.

B. P-Containing Four-Layer SLS Design

The electronic structure of a four-layer SLS structure with layer compositions and thicknesses 23.6 Å InAs/20 Å GaSb/23.6 Å InAs/60 Å $InP_{0.62}Sb_{0.38}$, and a 248.3-meV (5 μm) bandgap at 200 K is shown in Fig. 2. It is of a W-structure design [17] and is strain-balanced to a GaSb substrate. We compute an Auger coefficient $\gamma_{3\mathrm{hh}} = 7.9 \times 10^{-28}$ cm^6/s for this structure. Its optical absorption coefficient is plotted in Fig. 3 and compared with the two-layer design of the previous section and bulk HgCdTe. We see that the absorption is significantly stronger than that of the two-layer design and comparable to HgCdTe at its onset.

As described in Section IV, the dark currents of infrared photodiodes based on SLS and HgCdTe were compared by scaling the thickness of the SLS absorber layer to give the same αd product as for a 5-μm-thick HgCdTe absorber. The α and d values for 23.6 Å InAs/20 Å GaSb/23.6 Å InAs/60 Å $InP_{0.62}Sb_{0.38}$ are compared with those for HgCdTe in Table I. Note that the weaker absorption of the P-containing four-layer SLS relative to HgCdTe at $9\lambda_g/10$ means that this design requires a thicker absorber region than HgCdTe to produce the same quantum efficiency.

TABLE I
200 K OPTICAL PROPERTIES OF ABSORBERS AND ASSOCIATED ABSORBER LAYER THICKNESS d

	$Hg_{0.715}Cd_{0.285}Te$	23.6 Å InAs/ 20 Å GaSb/23.6 Å InAs/ 60 Å $InP_{0.62}Sb_{0.38}$ on GaSb (P-containing 4-layer SLS)
λ_g (μm)	5.01	4.99
α at wavelength $9\lambda_g/10$ (cm^{-1})	2335	1843
d (μm)	5.0	6.3

The computed minority carrier lifetimes are plotted in Fig. 4. We predict the longest recombination lifetimes for the P-containing four-layer SLS, p-type $Hg_{0.715}Cd_{0.285}Te$ and then n-type $Hg_{0.715}Cd_{0.285}Te$ having increasingly shorter lifetimes. The corresponding dark currents are presented in Fig. 5. For all doping choices, the lowest dark current is predicted for the 23.6 Å InAs/20 Å GaSb/23.6 Å InAs/60 Å $InP_{0.62}Sb_{0.38}$ SLS and the highest for n-type $Hg_{0.715}Cd_{0.285}Te$, with about 1.5 orders of magnitude between these two. Fig. 6 plots Rule 07 (a useful estimator for state-of-the-art HgCdTe dark current density) [18] together with the dark currents as predicted in Fig. 5 for 10^{15} cm^{-3} doping.

In summary, the consideration of a P-based electron–hole barrier layer of the SLS structure has resulted in a design that is predicted to yield ideal MWIR photodiodes with dark currents 35 times lower than those based on an n-type HgCdTe absorber

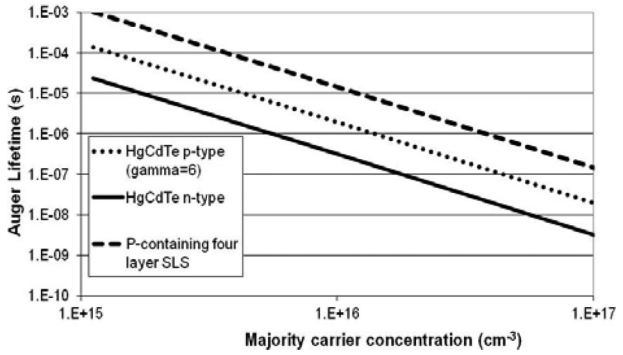

Fig. 4. Computed minority carrier lifetimes $\tau_{\min}$ of p- and n-type doped $Hg_{0.715}Cd_{0.285}Te$ (MCT) and the p-type 23.6 Å InAs/20 Å GaSb/23.6 Å InAs/60 Å $InP_{0.62}Sb_{0.38}$ SLS (P-containing four-layer SLS), all at 200 K.

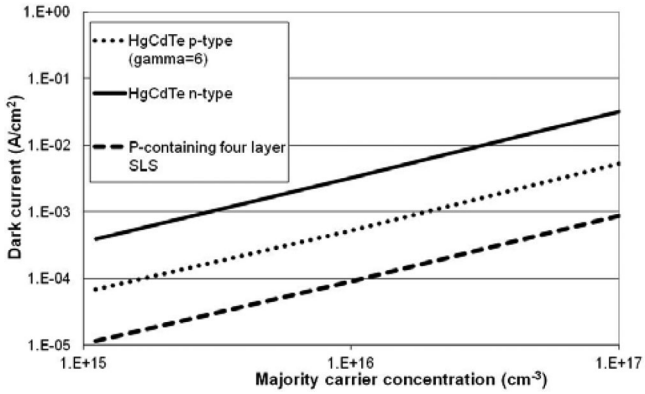

Fig. 5. Computed dark currents for diffusion-limited diodes with absorber layers consisting of the same materials as in Fig. 4 and absorber layer thicknesses as in Table I, all at 200 K.

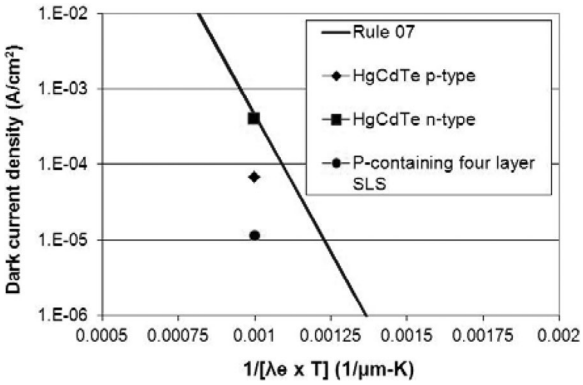

Fig. 6. Rule 07 (line) with specific dark current predictions for diffusion-limited diodes with absorber layers consisting of the same materials as in Fig. 4.

and six times lower than a p-type HgCdTe one for the same bandgap, temperature, and dopant concentration. Moreover, the needed absorber layer thickness is only about 25% greater than that of HgCdTe to produce the same quantum efficiency at a wavelength of 4.5 μm.

VI. Defect-Mitigation Strategy

Present-day Type-II SLS-based photodetectors remain defect-limited in their performance [19]. We propose here a defect-mitigation strategy that does not require the elimination of defects but rather limits the effectiveness of existing defects in mediating recombination. We note that this strategy applies to contributions to the photodiode dark current from defect-mediated generation and recombination in SLS-based absorber and depletion layers, unlike other strategies that reduce or eliminate dark current contributions arising from only depletion regions or surfaces [14], [19].

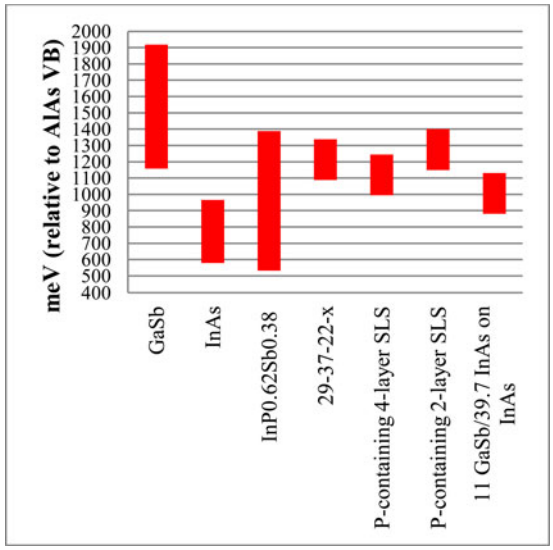

Fig. 7. 200-K bandgap positions of bulk GaSb, bulk InAs, bulk $InP_{0.62}Sb_{0.38}$ (one of the constituent layers of the P-containing four-layer SLS), and four Type-II SLS. "29–37. . ." refers to a 29 Å $InAs_{0.91}Sb_{0.09}$/37 Å GaSb/22 Å $InAs_{0.91}Sb_{0.09}$/23.2 Å GaSb SLS. The two P-containing SLS are described in Section V. "11 GaSb/39.7 InAs on InAs" is the only SLS considered in this paper that is on an InAs, rather than a GaSb substrate. All the SLS have 5-μm bandgaps at 200 K.

The strategy is based on the assumption that the current-limiting defects arise from states native to one or both of the component materials (GaSb and its alloys or InAs and its alloys). Adroit use of this proposed approach allows engineering the position of the energy gap of an SLS to a desired absolute energy range that ideally does not contain component material defect levels or at least results in shallow defects that are less effective in mediating Shockley–Read–Hall recombination. Fig. 7 shows the bandgaps of four SLS relative to bulk GaSb, bulk InAs, and bulk $InP_{0.62}Sb_{0.38}$ to demonstrate this concept. The absolute energy gap positions of the SLS were designed to have varying degrees of overlap with the bulk GaSb gap. We see that shallow donors or mid-gap defects in GaSb would be resonances in these SLS designs. Shallow acceptors in GaSb could become deep-level defects in the SLS; however, their exact position in the SLS gap (or outside of it) can be positioned by appropriate SLS design. A major conclusion is that it is possible to tune the absolute position of the energy gap of a 5-μm bandgap SLS at 200 K by design variation. This has implications with regard to the defects that mediate Shockley–Read–Hall recombination, namely a particular defect level may be a deleterious deep-level one in one design yet a less-harmful shallow one or even a resonance in another design. As such, when a particular defect level is discovered in a particular SLS design, other designs can

be generated using the tools presented in this paper with the same cutoff wavelength but positioning the same defect level either shallower or completely out of the gap, thereby diminishing its harmful effects on recombination lifetimes. We note that this strategy can be effective no matter what the origin of the defect (intrinsic or extrinsic), but it does require that those defect levels most deleterious to recombination lifetimes can be positioned outside of the SLS bandgap or at least near the band edges. This may be challenging if a particular defect produces multiple states that all readily mediate recombination and they are distributed over an energy range comparable to the SLS bandgap.

VII. Summary

We theoretically examined Type-II SLS structures with two-layer InGaSb/InPSb and four-layer InAs/GaSb/InAs/InPSb SLS periods for utilization as absorber layers of MWIR photon detectors. Among the studied designs, the lowest dark current in an ideal structure is predicted for a four-layer 23.6 Å InAs/20 Å GaSb/23.6 Å InAs/60 Å $InP_{0.62}Sb_{0.38}$ SLS. Its predicted ideal dark current is about 35 times lower than an n-type HgCdTe-based absorber and six times lower than a p-type HgCdTe one for the same bandgap, temperature, and dopant concentration. We also proposed a defect mitigation strategy that involves positioning the SLS gap in an energy range that avoids defect levels. This study points the need for future exploration of the many degrees of freedom offered in infrared SLS to optimize both intrinsic material properties and minimize the influence of defects

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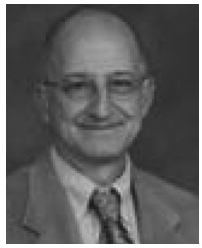

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